

Minimum uncertainty for antisymmetric wave functions

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Abstract

We study how the entropic uncertainty relation for position and momentum conjugate variables is minimized in the subspace of one-dimensional antisymmetric wave functions. Based partially on numerical evidence and partially on analytical results, a conjecture is presented for the sharp bound and for the minimizers. Conjectures are also presented for the corresponding sharp Hausdorff-Young inequality.

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Let ψ be in a square integrable function in \mathbb{R}^n , to represent the wave function of a quantum-mechanical particle, and let ρ be its normalized probability density, to wit, $\rho(x) = |\psi(x)|^2 / \|\psi\|_2^2$, where $\|\psi\|_p$ denotes the p -norm $(\int |\psi(x)|^p d^n x)^{1/p}$. The information entropy of ψ (or ρ) is defined as

$$S(\psi) = - \int \log(\rho(x)) \rho(x) d^n x. \quad (1)$$

It measures the localization of the state in configuration space. A high entropy implies a low spatial localization and vice versa. Likewise, one can consider the wave function in momentum space, defined by the Fourier transform of ψ , that is

$$(\mathcal{F}\psi)(x) = \int e^{2\pi i x y} \psi(y) d^n y \quad (2)$$

for ψ integrable. (The normalization of \mathcal{F} corresponds to using units $2\pi\hbar = 1$.) We will often use the notation $\tilde{\psi}$ for the Fourier transform of ψ . Again, its information entropy $S(\tilde{\psi})$ is a measure of its momentum space localization.

As shown by Hirschman [1] in one dimension and by Białynicki-Birula and Mycielski in the n -dimensional case [2], the basic uncertainty relations of position and momentum in quantum mechanics can be derived from the following sharp bound in $L^2(\mathbb{R}^n)$:

$$S(\psi) + S(\tilde{\psi}) \geq n(1 - \log 2). \quad (3)$$

Indeed, this inequality puts a bound on the maximum localization in phase space and, in particular, it can be shown to imply the uncertainty relations of Heisenberg (Weyl-Heisenberg inequality) [1,2]. As stressed by Deutsch [3], entropic uncertainty relations among observables are a more faithful expression of the quantum-mechanical uncertainty principle than the customary generalized Heisenberg relations. (See also [4–6] for further details and applications.)

The equality in (3) is reached by any Gaussian function and moreover these are the unique minimizers [7]. Since the Gaussian can be taken centered at the origin, the same sharp bound holds in the subspace of even functions. Less obvious is the value of the sharp

bound in the subspace spanned by the odd functions, i.e., $\psi(-x) = -\psi(x)$, as well as the form of the associated minimizing functions. Such question would arise, for instance, in the case of two electrons in a triplet spin state since the relative coordinate wave function must be odd. In this paper we will address this problem in the one dimensional case, $n = 1$. For future reference, we will denote the functional $S(\psi) + S(\tilde{\psi})$ by $\mathcal{S}(\psi)$ and the subspace of the odd functions in $L^2(\mathbb{R})$ by \mathcal{H}_- . Thus, we seek to find the infimum of \mathcal{S} in the space \mathcal{H}_- , and also to establish the form of the possible minimizers, or, more generally, of the minimizing sequences.

Quite likely the problem just raised is non trivial if treated in a fully rigorous mathematical manner. In 1957 it was noted by Hirschman (in the one dimensional case) that the l.h.s. of (3) is non negative; this result follows from the classical Hausdorff-Young inequality (see e.g. [8]), he then conjectured that the sharp bound was attained by Gaussian functions [1]. It was not until 1975 that Beckner [8], motivated by preliminary results of Babenko [9], established the necessary sharp version of Hausdorff-Young inequality from which Hirschman-Beckner inequality (3) immediately follows. On the other hand, the problem of finding sharp bounds in restricted classes of functions, such as linear subspaces, seems to have deserved less or not attention at all. Given the difficulty of the problem, we have adopted here an exploratory approach in order to gather “experimental” information on the minimizing function, namely, by numerically minimizing the entropy functional. From the point of view of rigorous mathematical results, this procedure can only yield upper bounds on the sharp bound, nevertheless it can provide useful insights and help to make reasonably founded conjectures on the form of the minimizers. Such conjectures are presented below.

Let us briefly describe the numerical procedure used. We have considered the expansion of the elements of $L^2(\mathbb{R})$ in terms of the orthonormal harmonic oscillator basis $\phi_n(x) = h_n(x)e^{-\pi x^2}$, where $h_n(x)$ are the associated Hermite polynomials. Thus $\psi(x) = \sum_{n=0}^{\infty} a_n \phi_n(x)$ in the mean. In this basis the Fourier transform takes the simple form $\tilde{\psi}(x) = \sum_{n=0}^{\infty} i^n a_n \phi_n(x)$. The entropy functional \mathcal{S} is then transformed into a function of the complex coefficients a_n and the problem consists in minimizing this function with respect to a_{2n+1} , $n = 0, 1, 2, \dots$,

keeping $a_{2n} = 0$ and $\sum_{n=0}^{\infty} |a_n|^2$ finite. To address this problem we actually consider the following N -dimensional subspace of \mathcal{H}_-

$$\psi(x) = \sum_{n=0}^{N-1} a_{2n+1} \phi_{2n+1}(x), \quad (4)$$

for N as large as possible, then make use of standard numerical algorithms to look for the minimum of $\mathcal{S}(\psi)$ in this space. The numerical minimization algorithms become less efficient as N increases, thus implying a maximum admissible value for N in practice. The largest space used was that corresponding to $N = 128$, which, of course, yielded the best (i.e., the lowest) entropy, namely, $\mathcal{S}(\psi) = 0.61370581$. This number, as well as the minimizing functions itself, is only very weakly dependent on the minimization method used (e.g. a steepest descend or a simplex algorithm), the precise value of N and the initial conditions used. Also, we have checked that the Gaussian minimum $1 - \log 2$ is correctly reproduced if even as well as odd functions are allowed. It turned out that imposing the conditions $\psi^* = \psi$ and $\tilde{\psi} = +i\psi$ did not result in an increase of the entropy. Analogous restrictions can be imposed on the Gaussian minimizer in the subspace of even functions. The minimizing function (for $N = 128$ and the above mentioned restrictions) is shown in Figure 1.

Motivated by the numerical results, we define the following two one-parameter families of functions,

$$\begin{aligned} \Phi_a(x) &= \sum_{n \in \mathbb{Z}} (-1)^n e^{-\pi a^2 x^2} e^{-\pi(x-n-\frac{1}{2})^2/a^2}, \\ \Phi'_a(x) &= \sum_{n \in \mathbb{Z}} (-1)^n e^{-\pi a^2 (n+\frac{1}{2})^2} e^{-\pi(x-n-\frac{1}{2})^2/a^2}, \end{aligned} \quad (5)$$

where the parameter a takes positive values. Note that Φ_a and Φ'_a are two unrelated functions; the symbol $'$ is used to distinguish them and it does not denote a derivative. Our preliminary ansatz is that the small a limit of Φ_a (or equivalently of Φ'_a) corresponds to a minimizer of \mathcal{S} in \mathcal{H}_- . Under this assumption, the numerical curve shown in Figure 1 would be a regularized approximation to the small a limit of Φ_a . In fact, the numerical curve coincides almost perfectly with Φ_a or Φ'_a for $a = 0.29$. The parameter a plays the role of a regulator in eqs. (5), similar to value of N in eq. (4).

For convenience we will refer to (Φ_a) and (Φ'_a) as sequences since it is always possible to choose a positive sequence (a_n) with $\lim_{n \rightarrow \infty} a_n = 0$ so that (Φ_{a_n}) is a sequence in the usual sense. Strictly speaking the limits as $a \rightarrow 0$ of the (Φ_a) or (Φ'_a) do not take place within $L^2(\mathbb{R})$, i.e. in norm. Indeed, their point-wise limit is 0 except at the points $x_n = n + \frac{1}{2}$, where they take the value 1, whereas their norms $(\|\Phi_a\|_2)$ and $(\|\Phi'_a\|_2)$ converge to $1/\sqrt{2}$, as will be shown below. On the other hand the limit of $(\|\Phi_a - \Phi'_a\|_2)$ is 0, thus both sequences (Φ_a) and (Φ'_a) become equivalent for small a .

We will introduce the following notation. Let V be a normed vector space, and let (x_a) and (y_a) be two sequences in V (in the sense $a \rightarrow 0$ and a taking positive values). We will say that they strongly approach each other if $\lim_{a \rightarrow 0} \|x_a - y_a\| = 0$, and this will be denoted by $x \equiv y$ or $x_a \equiv y_a$. Let us remark that the sequences are not assumed to be Cauchy sequences, hence nothing is implied for the limits of $\|x_{a_1} - x_{a_2}\|$ or $\|x_{a_1} - y_{a_2}\|$ as a_1 and a_2 independently approach 0. From the triangle inequality it follows that this is an equivalence relation. Furthermore, if $x_a \equiv y_a$, it follows that $\lim_{a \rightarrow 0} (\|x_a\| - \|y_a\|) = 0$, since $|\|x_a\| - \|y_a\|| \leq \|x_a - y_a\|$. With this notation $\Phi_a \equiv \Phi'_a$ in $L^2(\mathbb{R})$. This is proved in Lemma 1 below.

The word “limit” applied to the sequences (Φ_a) and (Φ'_a) is used here only in an improper sense. The strict statement, if correct, would be that (Φ_a) is a minimizing sequence in \mathcal{H}_- , that is, one that approaches the infimum of \mathcal{S} in \mathcal{H}_- . A calculation, to be discussed in more detail later, shows that $\lim_{a \rightarrow 0} \mathcal{S}(\Phi_a) = 2(1 - \log 2)$, therefore we formulate the following conjecture:

Conjecture 1. *The infimum of the functional \mathcal{S} in \mathcal{H}_- is $2(1 - \log 2)$.*

Our best numerical value for \mathcal{S} (0.61370581) is only slightly above $2(1 - \log 2)$ (0.61370564). Let us make some remarks on the form of the assumed minimizing sequence and its improper limit Φ_0 . Both Φ_a and Φ'_a are odd and real functions and moreover $\mathcal{F}\Phi_a = i\Phi'_a$ and vice versa, thus $\mathcal{F}\Phi_a \equiv i\Phi_a$ in $L^2(\mathbb{R})$ (and also point-wise). Φ_0 is formed by a set of localized states arranged antisymmetrically around 0 and distributed equidistantly through the real

line. The small scale structures (the so called ultraviolet region in physics) are narrow Gaussian functions, namely, $e^{-\pi(x-x_n)^2/a^2}$. Likewise, the large scale structure (infrared region) is a wide Gaussian function centered at the origin, i.e, $e^{-\pi a^2 x^2}$. We will refer to this overall arrangement as a singular “bi-Gaussian” function. As it will be shown below, the double Gaussian structure of the minimizer Φ_0 is directly responsible for the fact that $2(1 - \log 2)$ is twice the infimum of \mathcal{S} in $L^2(\mathbb{R})$, which is saturated by a (simple) Gaussian function. As we will recall in a moment, minimizing \mathcal{S} is equivalent to maximize the Fourier transform operator. For any linear operator from $L^p(\mathbb{R}^n)$ into $L^q(\mathbb{R}^n)$ with a Gaussian kernel, Lieb has shown that the (unrestricted) maximizer, if any, must be a Gaussian function [7]. The subspace \mathcal{H}_- does not contain such functions, yet it seems that nevertheless a kind of Gaussian, to wit, a bi-Gaussian function, is the maximizer also in this case. It is remarkable how even the seemingly simple constraint $\psi \in \mathcal{H}_-$ yields a quite unexpected result, which however is full of structure.

The sharp bound $n(1 - \log 2)$ on the entropy \mathcal{S} follows from computing the norm of the Fourier transform operator \mathcal{F} considered as a linear operator from the space $L^p(\mathbb{R}^n)$ into its dual $L^q(\mathbb{R}^n)$, with $p^{-1} + q^{-1} = 1$ and $1 < p \leq 2 \leq q$ [1]. Indeed, we can define a new functional as

$$\mathcal{S}_q(\psi) = -\log \left(\frac{\|\mathcal{F}\psi\|_q}{\|\psi\|_p} \right). \quad (6)$$

\mathcal{S}_q vanishes at $q = 2$, since \mathcal{F} is unitary in $L^2(\mathbb{R}^n)$. The functional \mathcal{S}_q is related to the \mathcal{S} by

$$\mathcal{S}(\psi) = 4 \left. \frac{d\mathcal{S}_q(\psi)}{dq} \right|_{q=2}, \quad (7)$$

where the derivative is a right derivative. Following Hirschman’s argument, let $K_q(V)$ denote the norm of the operator \mathcal{F} restricted to a subspace V of $L^p(\mathbb{R}^n)$, i.e.

$$\inf\{\mathcal{S}_q(\psi), \psi \in V\} = -\log K_q(V). \quad (8)$$

From eq. (7) and using $K_2(V) = 1$, it follows

$$\inf\{\mathcal{S}(\psi), \psi \in V\} = -4 \left. \frac{dK_q(V)}{dq} \right|_{q=2}. \quad (9)$$

As first proved by Beckner [8], the infimum in $L^p(\mathbb{R}^n)$ is reached by Gaussian functions and thus $K_q(L^p(\mathbb{R}^n)) = (p^{1/p}q^{-1/q})^{n/2}$. In view of Conjecture 1, it is natural to make the stronger assumption

Conjecture 2. *The norm of the linear operator \mathcal{F} from the space \mathcal{H}_-^p of odd functions of $L^p(\mathbb{R})$ into $L^q(\mathbb{R})$, with $1 < p \leq 2$, is $K_q(\mathcal{H}_-^p) = p^{1/p}q^{-1/q}$. Correspondingly, the infimum of \mathcal{S}_q in \mathcal{H}_-^p is $\frac{1}{q} \log q - \frac{1}{p} \log p$.*

Conjecture 1 follows from this one. A calculation to be detailed below shows that the sequences (Φ_a) and (Φ'_a) yield the value $\mathcal{S}_q = \frac{1}{q} \log q - \frac{1}{p} \log p$ as a goes to 0, thus, according to this conjecture, they are minimizing sequences also for \mathcal{S}_q in \mathcal{H}_-^p .

Conjectures 1 and 2 settle the point (or, more properly, open the question) of the infimum of \mathcal{S} and \mathcal{S}_q in \mathcal{H}_-^p . As noted, we do not expect a strict minimizer of \mathcal{S}_q to exist and we have instead to consider minimizing sequences, i.e. such that $\lim_{n \rightarrow \infty} \mathcal{S}_q(\psi_n) = \inf\{\mathcal{S}_q, \text{ in } \mathcal{H}_-^p\}$. To address this point and the related problem of uniqueness, and also to give further support to the conjectures, we will now turn to a more detailed study of the bi-Gaussian ansatz Φ_a and Φ'_a and their admissible generalizations.

Let D_0 denote the class of distributions, $d_0(x)$ of the form

$$d_0(x) = \sum_{n \in \mathbb{Z}} b_n \delta(x - x_n), \quad x_n = x_0 + nr, \quad |b_n| = b, \quad r, b > 0, \quad (10)$$

for some x_0 , r and b . Here $\delta(x)$ is Dirac's delta function. Further, let ψ_2 be a function in $L^p(\mathbb{R}^2)$. Then, for each $a > 0$ we will associate to ψ_2 two functions ψ_1 and ψ'_1 in $L^p(\mathbb{R})$ by means of the relations

$$\psi_1(x) = \int d_0(y) \psi_2\left(ax, \frac{x-y}{a}\right) dy = \sum_{n \in \mathbb{Z}} b_n \psi_2\left(ax, \frac{x-x_n}{a}\right), \quad (11)$$

$$\psi'_1(x) = \int d_0(y) \psi_2\left(ay, \frac{x-y}{a}\right) dy = \sum_{n \in \mathbb{Z}} b_n \psi_2\left(ax_n, \frac{x-x_n}{a}\right). \quad (12)$$

We will use the notations $\langle d_0, \psi_2 \rangle_a$ and $\langle d_0, \psi_2 \rangle'_a$ to denote the defining constructions of ψ_1 and ψ'_1 respectively. Rather than state the more general conditions on ψ_2 for the above definitions to make sense, we will restrict ψ_2 to the Schwartz space of fast decreasing $C^\infty(\mathbb{R}^2)$

functions, on which the tempered distributions are defined. This space will be denoted by \mathcal{T} , and will be considered as a subspace of $L^p(\mathbb{R}^2)$. It has several useful properties: it is dense in $L^p(\mathbb{R}^2)$, is invariant under Fourier transform, and their elements are sufficiently regular for our purposes, in particular, the defining series of ψ_1 and ψ'_1 exist and are absolutely and uniformly convergent for given a .

Both definitions are related by using either ax or ax_n as the first argument of ψ_2 . We will be interested throughout in the limit of small positive a . In this limit, and for each n , the terms $\psi_2(ax, (x - x_n)/a)$ and $\psi_2(ax_n, (x - x_n)/a)$ vanish unless $x - x_n$ is of order a , thus both definitions become equivalent. More precisely, they strongly approach each other as a goes to 0, i.e.

$$\langle d_0, \psi_2 \rangle_a \equiv \langle d_0, \psi_2 \rangle'_a \quad \text{in } L^p(\mathbb{R}). \quad (13)$$

This statement is meaningful since the normalizations of ψ_1 and ψ'_1 are well-defined; they have finite p -norm as a goes to 0. This is proved in Lemma 1 and Proposition 1 below.

Perhaps the best way of understanding the constructions ψ_1 and ψ'_1 is to consider the case of a separable function $\psi_2(x, y) = \alpha(x)\beta(y)$. The definition of ψ_1 corresponds to make a convolution of d_0 with $\beta(x/a)$ and then multiply by $\alpha(ax)$, whereas in ψ'_1 the multiplication is performed in the first place and the convolution is done next. In the limit of small a both operations commute, i.e., $\alpha(\beta * d_0) \equiv \beta * (\alpha d_0)$. The function α describes the large scale profile of the function, whereas β gives the small scale structure of ψ_1 . For arbitrary functions ψ_2 , which can always be considered as a linear combination of separable ones, those roles are played by $\psi_2(x, 0)$ and $\psi_2(0, x)$, respectively.

The bi-Gaussian ansatzs Φ_a and Φ'_a are of the form $\langle d_0, \psi_2 \rangle_a$ and $\langle d_0, \psi_2 \rangle'_a$ with

$$d_0(x) = \sum_{n \in \mathbb{Z}} (-1)^n \delta(x - n - \frac{1}{2}), \quad (14)$$

$$\psi_2(x, y) = \exp(-\pi(x^2 + y^2)), \quad (15)$$

i.e. $b_n = (-1)^n$ and $x_n = n + \frac{1}{2}$.

The small a limit of ψ_1 or ψ'_1 does not take place in $L^p(\mathbb{R})$, nevertheless, after an appropriate renormalization, there is a weak limit as a distribution, namely

$$\lim_{a \rightarrow 0} \frac{1}{a} \psi_1(x) = \lim_{a \rightarrow 0} \frac{1}{a} \psi'_1(x) = K d_0(x), \quad (16)$$

where the constant $K = \int \psi_2(0, x) dx$. This follows from considering the integrals $\int \psi_1(x) f(x) dx$ or $\int \psi'_1(x) f(x) dx$ for an arbitrary test function f , after the change of variables $x \rightarrow ax + y$.

Let us compute the p -norm of ψ_1 in the limit $a \rightarrow 0$. Since in this limit the overlap among different terms of the defining series of ψ_1 is negligible, for each value of x at most one term of the series is relevant. This can be formulated as follows. For given d_0 in D_0 and each integer n , let I_n be interval $[x_n - \frac{1}{2}r, x_n + \frac{1}{2}r)$ and let $\varphi_n(x)$ denote the characteristic function of I_n . Then

$$\hat{\psi}_1(x) = \sum_{n \in \mathbb{Z}} b_n \psi_2\left(ax, \frac{x - x_n}{a}\right) \varphi_n(x), \quad \hat{\psi}'_1(x) = \sum_{n \in \mathbb{Z}} b_n \psi_2\left(ax_n, \frac{x - x_n}{a}\right) \varphi_n(x) \quad (17)$$

represent the truncated functions, obtained keeping only the relevant n for each x , i.e., such that $x \in I_n$.

The functions ψ_1 , ψ'_1 and their truncated versions are all equivalent:

Lemma 1. *Let $\psi_2 \in \mathcal{T}$, $d_0 \in D_0$ and $p \geq 1$, then $\psi_1 \equiv \psi'_1 \equiv \hat{\psi}_1 \equiv \hat{\psi}'_1$ in $L^p(\mathbb{R})$.*

The proof is given in the Appendix.

We can now compute the p -norms of ψ_1 in the limit of small a .

Proposition 1. *Let $\psi_2 \in \mathcal{T}$, $d_0 \in D_0$ and $p \geq 1$, then*

$$\lim_{a \rightarrow 0} \|\psi_1\|_p = \lim_{a \rightarrow 0} \|\psi'_1\|_p = \frac{b}{r^{1/p}} \|\psi_2\|_p. \quad (18)$$

Proof. Due to the previous lemma, it is enough to compute $\lim_{a \rightarrow 0} \|\hat{\psi}'_1\|_p$.

$$\begin{aligned} \|\hat{\psi}'_1\|_p^p &= b^p \sum_{n \in \mathbb{Z}} \int_{I_n} |\psi_2(ax_n, (x - x_n)/a)|^p dx \\ &= b^p a \sum_{n \in \mathbb{Z}} \int_{-r/2a}^{r/2a} |\psi_2(ax_n, x)|^p dx. \end{aligned} \quad (19)$$

Due to Lemma 1, the limits of the integral can be extended to $\pm\infty$. Next, we can use that for a Riemann integrable function f , $\int f(x) dx = \lim_{h \rightarrow 0} \sum_{n \in \mathbb{Z}} h f(x_0 + hn)$. Thus,

$$\lim_{a \rightarrow 0} \|\hat{\psi}'_1\|_p^p = \frac{b^p}{r} \int |\psi_2(y, x)|^p dx dy. \quad (20)$$

This proves the proposition.

Corollary 1. *For $\psi_2, \phi_2 \in \mathcal{T}$, $d_0 \in D_0$ and $p \geq 1$, $\langle d_0, \psi_2 \rangle_a \equiv \langle d_0, \phi_2 \rangle_a$ in $L^p(\mathbb{R})$ if and only if $\psi_2 = \phi_2$.*

A straightforward calculation shows that the Fourier transforms of ψ_1 and ψ'_1 are related to that of ψ_2 as

$$\mathcal{F}\langle d_0, \psi_2 \rangle_a = \langle \tilde{d}_0, T\tilde{\psi}_2 \rangle'_a, \quad \mathcal{F}\langle d_0, \psi_2 \rangle'_a = \langle \tilde{d}_0, T\tilde{\psi}_2 \rangle_a, \quad (21)$$

where T denotes the transposition operator, $T\psi_2(x, y) = \psi_2(y, x)$.

In order to proceed, we will consider admissible only the distributions d_0 in D_0 whose Fourier transform $\tilde{d}_0(x)$ is again in the class D_0 , that is

$$\tilde{d}_0(x) = \sum_{n \in \mathbb{Z}} \tilde{b}_n \delta(x - \tilde{x}_n), \quad \tilde{x}_n = \tilde{x}_0 + n\tilde{r}, \quad |\tilde{b}_n| = \tilde{b}, \quad (22)$$

for some \tilde{x}_0, \tilde{r} and \tilde{b} . The admissible distributions span the space $D_0^* := D_0 \cap \mathcal{F}^{-1}D_0$. Then, recalling that \mathcal{F} is a bijection in \mathcal{T} , Lemma 1 and Proposition 1 apply to $\tilde{\psi}_1$ and $\tilde{\psi}'_1$. This immediately leads to

Proposition 2. *For $\psi_2 \in \mathcal{T}$, $d_0 \in D_0^*$ and $1 \leq p \leq 2$, $p^{-1} + q^{-1} = 1$,*

$$\lim_{a \rightarrow 0} \mathcal{S}_q(\psi_1) = \mathcal{S}_q(\psi_2) + C_q, \quad C_q = \log \left(\frac{b \tilde{r}^{1/q}}{\tilde{b} r^{1/p}} \right), \quad (23)$$

$$\lim_{a \rightarrow 0} \mathcal{S}(\psi_1) = \mathcal{S}(\psi_2) + C, \quad C = -\log(r\tilde{r}). \quad (24)$$

In both cases, the first term depends only on ψ_2 and the second one only on d_0 . Furthermore, if $\psi_2(x, y)$ happens to be separable as $\alpha(x)\beta(y)$, the entropies also split as the sum of the entropies corresponding to the infrared part α plus the ultraviolet part β . Let us denote by $\mathcal{H}(d_0)$ the (improper) subspace of $L^2(\mathbb{R})$ spanned by the functions ψ_1 , for given d_0 , in the limit of small a . From these formulae follows that the minimum entropy in $\mathcal{H}(d_0)$ corresponds to those ψ_1 associated to a Gaussian ψ_2 , i.e. ψ_1 must be a bi-Gaussian function. Therefore,

Corollary 2. *Under the same assumptions as in Proposition 2, the following bounds are sharp in $\mathcal{H}(d_0)$ and are attained by ψ_2 Gaussian.*

$$\lim_{a \rightarrow 0} \mathcal{S}_q(\psi_1) \geq \frac{1}{q} \log q - \frac{1}{p} \log p + C_q, \quad (25)$$

$$\lim_{a \rightarrow 0} \mathcal{S}(\psi_1) \geq 2(1 - \log 2) + C. \quad (26)$$

On the other hand, $\mathcal{S}_q(\psi_1)$ is bounded from below by its infimum in $L^p(\mathbb{R})$, namely, $\frac{1}{2q} \log q - \frac{1}{2p} \log p$, hence it follows that any d_0 in D_0^* must satisfy the following inequalities

$$\begin{aligned} C_q &\geq -\frac{1}{2q} \log q + \frac{1}{2p} \log p \quad (1 < p \leq 2), \\ C &\geq -1 + \log 2. \end{aligned} \quad (27)$$

The distribution d_0 in eq. (14) satisfies $\mathcal{F}d_0 = id_0$. This is easily proved using Poisson's summation formula $\sum_{n \in \mathbb{Z}} \exp(i2\pi nx) = \sum_{n \in \mathbb{Z}} \delta(x + n)$. Thus this d_0 is admissible and the sharp bounds apply with $r = \tilde{r} = b = \tilde{b} = 1$, i.e., with $C_q = C = 0$. This is consistent with Conjecture 2 since Φ_a is a bi-Gaussian odd function. Moreover, $\tilde{\Phi}_a = i\Phi'_a$ and $\tilde{\Phi}'_a = i\Phi_a$. This follows from $\tilde{\psi}_2(x, y) = \psi_2(y, x)$ for ψ_2 in eq. (15).

As a further check of Conjecture 2, let us show that, for the admissible d_0 , the functional \mathcal{S}_q is stationary at ψ_1 , when ψ_1 is a singular bi-Gaussian function.

Lemma 2. *Let $d_0 \in D_0^*$, then $b^2/r = \tilde{b}^2/\tilde{r}$.*

Proof. This follows from using that \mathcal{F} is unitary in $L^2(\mathbb{R}^n)$, thus, for any $\psi_2 \in \mathcal{T}$,

$$\frac{b^2}{r} \|\psi_2\|_2^2 = \lim_{a \rightarrow 0} \|\psi_1\|_2^2 = \lim_{a \rightarrow 0} \|\tilde{\psi}_1\|_2^2 = \frac{\tilde{b}^2}{\tilde{r}} \|T\tilde{\psi}_2\|_2^2 = \frac{\tilde{b}^2}{\tilde{r}} \|\psi_2\|_2^2. \quad (28)$$

Proposition 3. *Let ψ_2 be a Gaussian function, and $d_0 \in D_0^*$, then \mathcal{S} and \mathcal{S}_q are stationary at $\psi_1 = \langle d_0, \psi_2 \rangle_a$ in the limit $a \rightarrow 0$.*

Proof. Let us consider a first order variation of ψ . The first order variation of \mathcal{S}_q in $L^p(\mathbb{R}^n)$ is easily computed from its definition, yielding

$$\delta \mathcal{S}_q(\psi) = \text{Re} \int \delta \psi^*(x) \left(G_p - \mathcal{F}^{-1} G_q \mathcal{F} \right) \psi(x) d^n x, \quad (29)$$

where we have introduced the non linear operator G_s

$$G_s \psi(x) = \frac{\psi(x) |\psi(x)|^{s-2}}{\|\psi\|_s^s}. \quad (30)$$

Since any Gaussian function is a minimizer of \mathcal{S}_q , it follows that $(G_p - \mathcal{F}^{-1} G_q \mathcal{F}) \psi_2$ vanishes identically when ψ_2 is Gaussian. On the other hand, since ψ_1 bi-Gaussian is a minimizer in the subspace $\mathcal{H}(d_0)$, $\delta \mathcal{S}_q(\psi_1)$ will also vanish if the variation $\delta \psi^*$ is in this subspace. What has to be proved is that in fact $\delta \mathcal{S}_q(\psi_1)$ vanishes under arbitrary variations, in the limit of small a . This is equivalent to prove that $(G_p - \mathcal{F}^{-1} G_q \mathcal{F}) \psi_1$ vanishes when ψ_1 is a singular bi-Gaussian function. From arguments entirely similar to those used to establish Proposition 1, it follows

$$G_s \langle d_0, \psi_2 \rangle_a \equiv \frac{r}{b^2} \langle d_0, G_s \psi_2 \rangle_a, \quad (31)$$

from where it is finally obtained

$$(G_p - \mathcal{F}^{-1} G_q \mathcal{F}) \langle d_0, \psi_2 \rangle_a \equiv \left\langle d_0, \left(\frac{r}{b^2} G_p - \frac{\tilde{r}}{\tilde{b}^2} \mathcal{F}^{-1} G_q \mathcal{F} \right) \psi_2 \right\rangle_a. \quad (32)$$

Now, from Lemma 2, r/b^2 equals \tilde{r}/\tilde{b}^2 ; this quantity factors out and the right-hand side vanishes for ψ_2 Gaussian. This completes the proof.

Let us note that the inequalities (27), as well as Lemma 2 are statements on the space D_0^* only, independent of the construction $\langle d_0, \psi_2 \rangle_a$. This construction, however, defines a regularization of d_0 which has proven useful to establish properties in D_0^* .

It is also interesting to note that a similar construction to that of Φ_a can be carried out for the space of even functions, using the same ψ_2 given in eq. (15) and the distribution

$$d_0(x) = \sum_{n \in \mathbb{Z}} \delta(x - n), \quad (33)$$

which satisfies $\tilde{d}_0 = d_0$. All the previous arguments apply here and the same sharp bound for \mathcal{S}_q in $\mathcal{H}(d_0)$ is obtained as for the case of d_0 odd. Of course, the corresponding bi-Gaussian is known not to be a minimizer of the even functions subspace and at most it can be a relative minimum.

An immediate question is that of the uniqueness of the minimizing sequence. To study this point we have first to consider the symmetries of \mathcal{S} and \mathcal{S}_q . In $L^2(\mathbb{R}^n)$, the functional \mathcal{S} is

invariant under: (i) multiplication by a non-vanishing complex constant, $\psi(x) \mapsto \lambda\psi(x)$, (ii) affine regular transformations, $\psi(x) \mapsto \psi(Ax + b)$, (iii) complex conjugation $\psi(x) \mapsto \psi^*(x)$, and (iv) Fourier transform, $\psi(x) \mapsto \tilde{\psi}(x)$. The functional \mathcal{S}_q in $L^p(\mathbb{R}^n)$ is invariant under the transformations (i)-(iii) above, whereas under Fourier transform it satisfies $\mathcal{S}_p(\mathcal{F}\psi) = -\mathcal{S}_q(\psi)$, provided the corresponding norms exist. In \mathcal{H}_-^p translation invariance does not exist and linear transformations consist only of dilatations. The improper minimizer Φ_0 is invariant under complex conjugation and Fourier transform but breaks dilatation and normalization invariances (as also does any non trivial function in $L^2(\mathbb{R}^n)$). In physics language, these two symmetries are spontaneously broken. A similar statement can be made for the Gaussian minimizers in $L^p(\mathbb{R}^n)$. Let us remark, however, that the group of symmetries generated by transformations (i)-(iv) does not act transitively on the set of minimizers of \mathcal{S} in $L^2(\mathbb{R})$, since complex (rather than real) affine transformations would be needed to connect two arbitrary Gaussian functions. Likewise, the previous symmetries applied to Φ_0 do not exhaust the set of minimizers, and in fact the symmetry group in $\mathcal{H}(d_0)$ is even larger; e.g. two independent dilatations applied to d_0 and ψ_2 still define an symmetry transformation which acts effectively on $\mathcal{H}(d_0)$ (always meaning in the limit of small a for which $\mathcal{H}(d_0)$ has been defined).

In passing, note that under a dilatation $d_0(x) \rightarrow \mu^{1/2}d_0(\mu x)$, (μ positive), the quantities b , \tilde{b} , r and \tilde{r} scale as $\mu^{-1/2}b$, $\mu^{1/2}\tilde{b}$, $\mu^{-1}r$ and $\mu\tilde{r}$, respectively. Thus the quantities r/b^2 , C_q and C are dilatation invariant, as they should.

As noted above, the sequence (Φ_a) is not convergent in $L^p(\mathbb{R})$ and it cannot be made convergent by a suitable (a -dependent) renormalization of Φ_a since its weak limit is the singular distribution d_0 . Thus it is not a Cauchy sequence; two elements Φ_{a_1} and Φ_{a_2} need not be near each other in the strong topology, even for arbitrarily small values of a_1 and a_2 . That is, the sequence does not even approach itself in the mean and hence a precise definition is needed to state that some other minimizing sequence must approach this one. Besides, note that given a minimizing sequence, one can apply independent arbitrary symmetry transformations for each value of a and still have a minimizing sequence. This implies that

a minimizing sequence needs not approach strongly (Φ_a) or more generally $(\langle d_0, \psi_2 \rangle_a)$ for fixed (i.e. a -independent) d_0 and ψ_2 .

The numerical calculation shows that the infimum in \mathcal{H}_- can be achieved in the subspace $\mathcal{F} = +i$, whereas that corresponding to the subspace $\mathcal{F} = -i$ is larger. This suggests that Fourier transform invariance is not spontaneously broken, that is, that after an appropriate dilatation, the minimizer can be brought to the space $\mathcal{F} = +i$ (note that \mathcal{F} is not invariant under dilatations). This is similar to the problem of minimizing \mathcal{S} in $L^2(\mathbb{R})$; a minimizer (a Gaussian) is not necessarily an even function, but it can be brought to one after a suitable translation. In the case of \mathcal{H}_-^p , not existing a true minimizer, it is important to specify in which sense the minimizer must satisfy the condition $\mathcal{F}\psi = +i\psi$ (assuming our conjecture of unbroken Fourier transform invariance to hold). One can expect that the condition is satisfied in the weak sense. This is consistent with the fact that $a^{-1}\psi_1$ weakly converges to d_0 . It cannot be expected, however, to hold in strong sense for an arbitrary minimizing sequence. This can be seen noting that every centered Gaussian ψ_2 , together with d_0 in eq. (14), would yield a minimizing sequence in \mathcal{H}_-^p . By a centered Gaussian, it is meant a function of the form $\psi_2(x, y) = N \exp(-\frac{1}{2}Ax^2 - \frac{1}{2}By^2 - Cxy)$, where N , A , B and C are complex numbers, N is non vanishing and the real part of $\frac{1}{2}Ax^2 + \frac{1}{2}By^2 + Cxy$ is a positive definite quadratic form. In this case $\psi_1 = \langle d_0, \psi_2 \rangle_a$ is an antisymmetric bi-Gaussian function. Then, $\tilde{\psi}_1' - i\psi_1 = i\langle d_0, T\tilde{\psi}_2 - \psi_2 \rangle_a$, whose norm (from Corollary 1) does not go to 0 unless $\tilde{\psi}_2 = T\psi_2$, and this equality does not hold for an arbitrary centered Gaussian ψ_2 .

Another consideration follows from noting that the information entropy S of d_0 is undefined; each single delta function has entropy minus infinity since they correspond to a maximal localization, however, the fact that this localization can occur in any of the points x_n with equal probability adds a plus infinity to the entropy yielding a undefined value. It follows that the value of \mathcal{S} or \mathcal{S}_q for a sequence in $\mathcal{H}(d_0)$ depends not only on its weak limit, d_0 , but also on the particular shape of the functions: the true minimizer must be Gaussian-like.

Perhaps it will be useful to illustrate the situation with an example. Consider the minimization of the functional $F(\psi) = F_0(\psi) + F_1(\psi)$ on $L^2(\mathbb{R})$, where

$$F_0(\psi) = S(\psi) - \frac{1}{2} \log \langle (x - \langle x \rangle_\psi)^2 \rangle_\psi, \quad F_1(\psi) = \langle (x - \langle x \rangle_\psi)^2 \rangle_\psi, \quad (34)$$

and $\langle f(x) \rangle_\psi$ means $\int f(x) \rho(x) dx$. F_0 has been adjusted so that it is invariant under dilatations, whereas, F_1 is minimized by functions as narrow as possible. Therefore, we can proceed by classifying the space of functions by their value of F_1 , and choose the minimizer of F_0 in each class. A simple calculation, using Lagrange multipliers, shows that the minimizer is a Gaussian located anywhere and with arbitrary normalization and a well-defined width a . This gives $F_1 = a^2/2\pi$ and $F_0 = \frac{1}{2} + \frac{1}{2} \log 2\pi$. Next, in order to minimize F_1 , we should take $a \rightarrow 0$. The infimum of F is then $\frac{1}{2} + \frac{1}{2} \log 2\pi$. The absolute minimizer does not exist in $L^2(\mathbb{R})$, but a minimizing sequence must approach in some sense the sequence $\psi_a(x) = \exp(-\pi x^2/2a^2)$ in the limit $a \rightarrow 0$, modulo normalization and location. Furthermore, the corresponding probability density $\rho_a(x)$ must approach the distribution $\delta(x)$, again modulo translations.

After these considerations, we will state our conjecture on the form of the minimizer of \mathcal{S}_q in \mathcal{H}_-^p . Essentially, it is that a minimizer must necessarily be a singular bi-Gaussian in the space $\mathcal{F} = +i$ (in the weak sense) and modulo dilatations. To put this conjecture in precise terms, let d_0 denote precisely the distribution in eq. (14) and let $\psi^\mu(x)$ denote $\psi(\mu x)$, where $\mu > 0$ and $\psi \in L^p(\mathbb{R})$.

Conjecture 3. *Let (ψ_a) be a minimizing sequence for \mathcal{S}_q in \mathcal{H}_-^p (in the sense of $a \rightarrow 0$ and the parameter a taking positive values). Then, (a) there is a sequence of positive numbers (μ_a) and a sequence of complex numbers (λ_a) such that $(\lambda_a \psi_a^{\mu_a})$ converges weakly to d_0 . According to (a), let us assume, without loss of generality, that (ψ_a) has this property with $\mu_a = 1$ and that it is normalized to unity, $\|\psi_a\|_p = 1$. Then, (b) there is a sequence of centered Gaussian functions $(\psi_{2,a})$ such that the sequence $(\langle d_0, \psi_{2,a} \rangle_a)$ strongly approaches (ψ_a) , that is, $\lim_{a \rightarrow 0} \|\psi_a - \langle d_0, \psi_{2,a} \rangle_a\|_p = 0$.*

It is clear that this conjecture is stronger than Conjecture 2. It states that conditions (a) and (b) are necessary for a minimizing sequence. On the other hand, assuming Conjecture 2, they are sufficient: first note that $\psi_a \equiv \phi_a$ in $L^p(\mathbb{R})$ guarantees $\tilde{\psi}_a \equiv \tilde{\phi}_a$ in $L^q(\mathbb{R})$, and thus if $\|\psi_a\|_p$ is normalized to unity and $\|\tilde{\psi}_a\|_q$ has a finite non zero limit, $\lim_{a \rightarrow 0} (\mathcal{S}_q(\psi_a) - \mathcal{S}_q(\phi_a)) = 0$. Further, Proposition 1 was proved assuming $\psi_2(x, y)$ to be independent of a . The danger with an a -dependent $\psi_{2,a}$ is that, if $a^2 \langle y^2 \rangle_{\psi_{2,a}}$ or $a^{-2} \langle x^2 \rangle_{\psi_{2,a}}$ do not go to 0 for small a , the various terms in the series of ψ_1 or $\tilde{\psi}_1$, respectively, overlap and the proposition does not apply. This danger is avoided by condition (a) since ψ_a is assumed to approach d_0 which consists of well separated Dirac deltas.

In conclusion, we have presented a set of conjectures on the infimum and on the minimizers of the functionals \mathcal{S} and \mathcal{S}_q in the space of odd one-dimensional functions. They are based on information obtained through a simple-minded direct approach, namely, a numerical minimization. This cannot be made into anything rigorous, since the numerical procedure might lead to a relative minimum, rather than to the absolute one, however this possibility seems quite unlikely to us since the numerical result has been checked to be stable against details of the calculation, including changes in the initial conditions chosen for the minimization.

Although at first sight the numerical result in Figure 1 seems to be rather irregular, we have hopefully shown in this work that in fact it is plenty of structure and regularity. The space $\mathcal{H}(d_0)$ has proven to have nice properties directly inherited from the map $d_0 \otimes L^p(\mathbb{R}^2)$ into $L^p(\mathbb{R})$. The numerical value of the infimum of \mathcal{S} in \mathcal{H}_- has been understood as an approximation to twice the absolute infimum in $L^2(\mathbb{R})$ and the numerical minimizer has been understood as a (singular) double Gaussian structure. Gaussian functions seem to dominate the entropy minimization problem both in the whole space and in the odd functions subspace. Likely, these regularities will open the way for a rigorous treatment of the problem studied here.

APPENDIX A: PROOF OF LEMMA 1.

Let us begin by proving $\psi'_1 \equiv \widehat{\psi}'_1$. For $p \geq 1$, $\|\cdot\|_p$ is a norm, hence, due to the triangle inequality

$$\|\psi'_1 - \widehat{\psi}'_1\|_p \leq b \sum_{\substack{n,m \\ m \neq n}} \left(\int_{I_m} |\psi_2(ax_n, (x - x_n)/a)|^p dx \right)^{1/p}. \quad (\text{A1})$$

By assumption ψ_2 is bounded and fast decreasing at infinity, thus for any s and t positive, there is a positive K such that $|\psi_2(x, y)| \leq K(1 + x^2)^{-s}|y|^{-t}$. Also, for $x \in I_m$, $|x - x_n| \geq r(|n - m| - \frac{1}{2})$. Therefore, for $s > 1/2$ and $t > 1$

$$\begin{aligned} \|\psi'_1 - \widehat{\psi}'_1\|_p &\leq bKa^t \sum_n (1 + a^2x_n^2)^{-s} \sum_{m \neq n} \left(\int_{I_m} |x - x_n|^{-tp} dx \right)^{1/p} \\ &\leq bKr^{1/p-t} a^t \sum_n (1 + a^2x_n^2)^{-s} \sum_{m \neq n} \left(|n - m| - \frac{1}{2} \right)^{-t}, \\ &= 2bKr^{1/p-t} a^t \sum_{m \geq 1} \left(m - \frac{1}{2} \right)^{-t} \sum_{n \in \mathbb{Z}} (1 + a^2x_n^2)^{-s} \\ &\leq K' a^{t-1}. \end{aligned} \quad (\text{A2})$$

In the last inequality we have used that the series on n is of order a^{-1} since $(1 + x^2)^{-s}$ is Riemann integrable and the x_n are equidistantly distributed. The proof of $\psi_1 \equiv \widehat{\psi}_1$ is analogous.

Since \equiv is an equivalence relation, it remains only to show that $\widehat{\psi}_1 \equiv \widehat{\psi}'_1$.

$$\begin{aligned} \|\widehat{\psi}_1 - \widehat{\psi}'_1\|_p^p &= b^p \sum_{n \in \mathbb{Z}} \int_{I_n} \left| \psi_2(ax, (x - x_n)/a) - \psi_2(ax_n, (x - x_n)/a) \right|^p dx \\ &\leq b^p a \sum_{n \in \mathbb{Z}} \int \left| \psi_2(ax_n + a^2x, x) - \psi_2(ax_n, x) \right|^p dx. \end{aligned} \quad (\text{A3})$$

Again, $\partial\psi_2(y, x)/\partial y$ is a fast decreasing function, thus, choosing $s > 1/2$ and $t > 1$,

$$\begin{aligned} \left| \psi_2(y + a^2x, x) - \psi_2(y, x) \right| &\leq \left| \int_y^{y+a^2x} |\partial_z \psi_2(z, x)| dz \right| \\ &\leq \left| \int_y^{y+a^2x} \frac{K}{(1 + x^2)^t (1 + z^2)^s} dz \right| \\ &\leq \frac{a^2 K |x|}{(1 + x^2)^t (1 + y^2)^s}. \end{aligned} \quad (\text{A4})$$

$$\begin{aligned}
\|\widehat{\psi}_1 - \widehat{\psi}'_1\|_p^p &\leq b^p K^p a^{2p+1} \int \frac{|x|^p}{(1+x^2)^{tp}} dx \sum_{n \in \mathbb{Z}} \frac{1}{(1+(ax_n)^2)^{sp}} \\
&\leq K' a^{2p}
\end{aligned} \tag{A5}$$

This completes the proof of the lemma. Note that the conditions imposed on ψ_2 are far more restrictive than actually needed in the proof.

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FIGURES

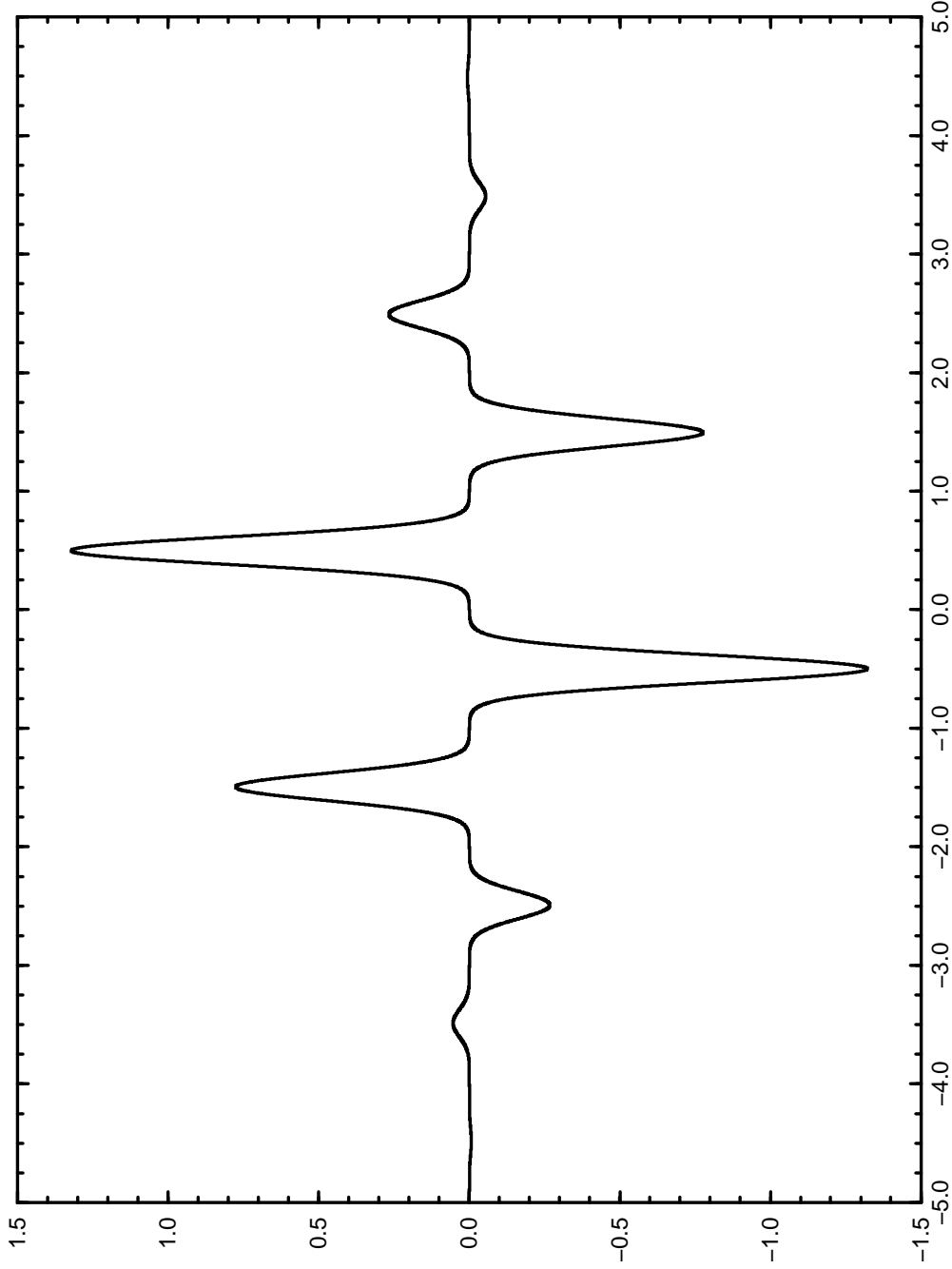


FIG. 1. Best minimizer of \mathcal{S} obtained through a 128-dimensional approximation to \mathcal{H}_- (cf. eq. (4)). The function is purely real and also satisfies $\tilde{\psi} = +i\psi$. The corresponding value of \mathcal{S} is 0.61370581.